Academic/DP Lab Alliance

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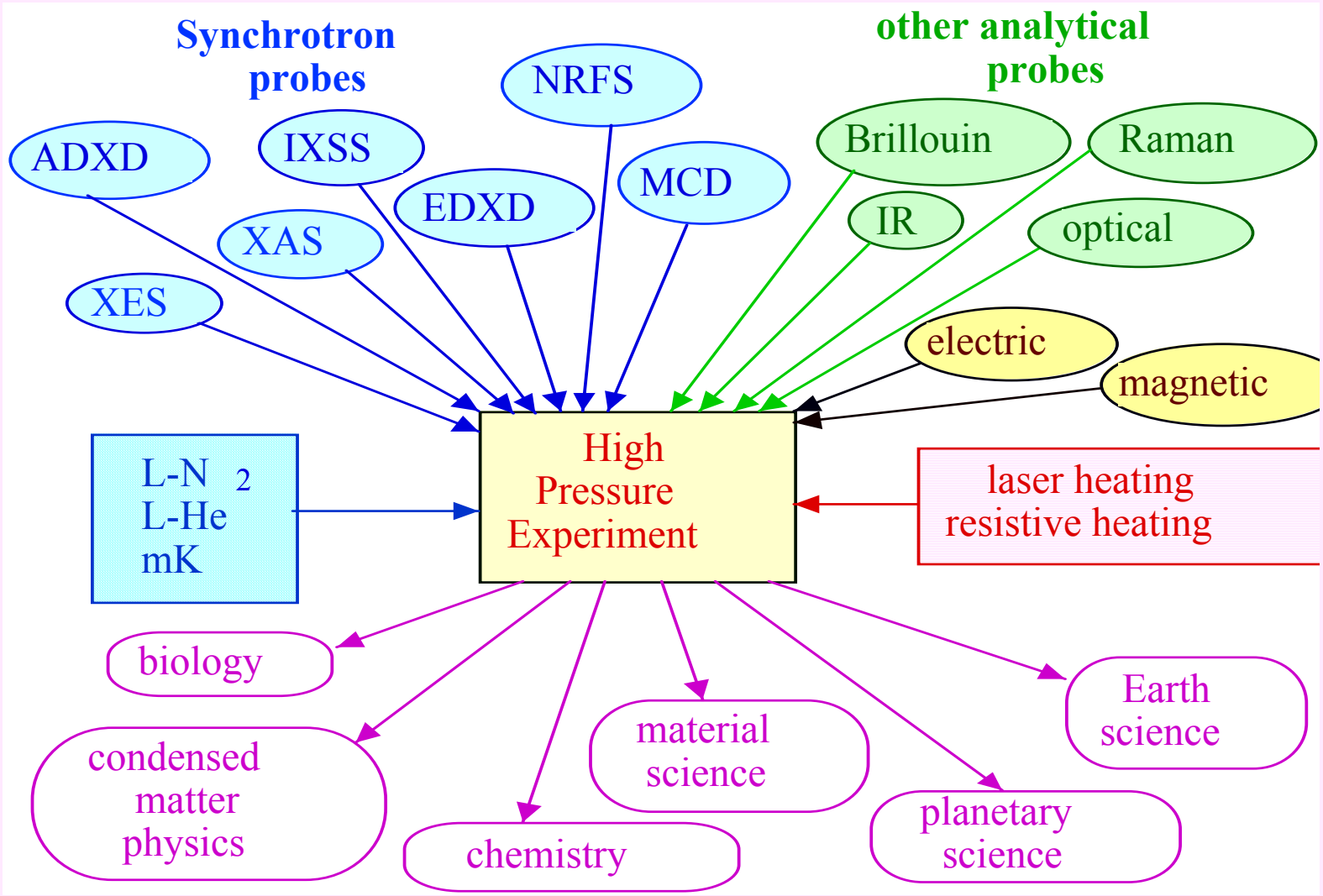
OUTLINE

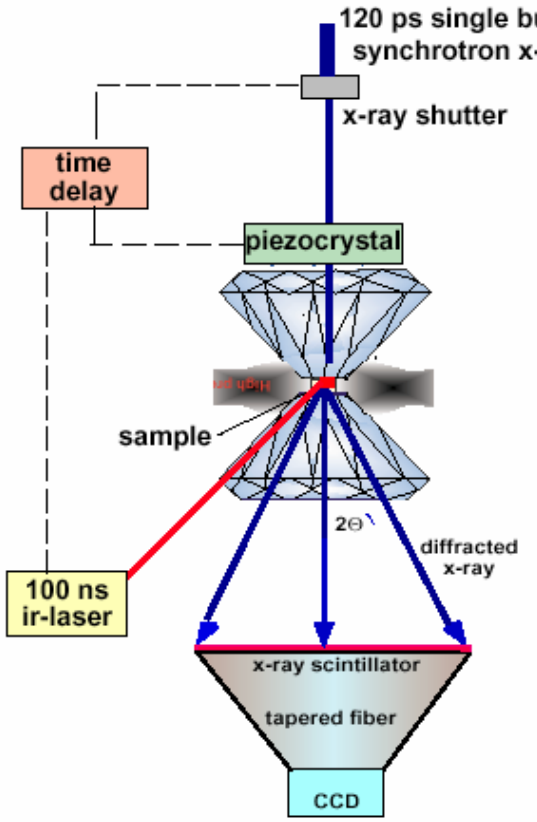
- Introduction
- Academic/DP Lab synergy in high-pressure research
- Interactions with classified research
- Key to successful collaboration
  - Clearly define boundaries
  - Overcome obstacles
  - Establish special programs and mechanisms

Academic/DP Lab Synergy
Examples: High-Pressure Research

- Development of high-pressure technology needs the broad expertise of academics and the focus of DP programs.
- Academics study the basics physics and deep Earth geophysics of transition elements under compression which are applicable to actinide programs at DP Lab.
- Academics study the novel high-pressure chemistry of simple molecular compounds which are relevant to high energitic materials for Stockpile Stewardship Program.
- Academics and DP Lab scientists pool their funds to build high-pressure synchrotron facilities at DOE-BES labs.

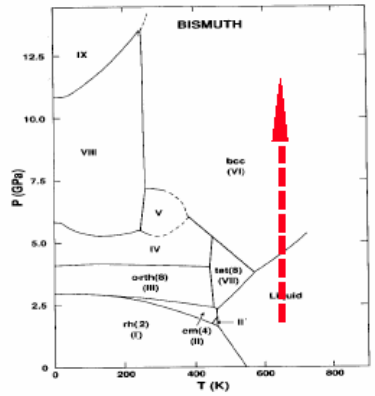

Synchrotron probes
other analytical probes
ADXD
IXSS
NRFS
EDXD
MCD
XAS
XES
Brillouin
Raman
IR
optical
electric
magnetic
L-N 2
L-He
mK
High Pressure Experiment
laser heating
resistive heating
biology
condensed matter physics
chemistry
material science
planetary science
Earth science

Real-time x-ray diffraction



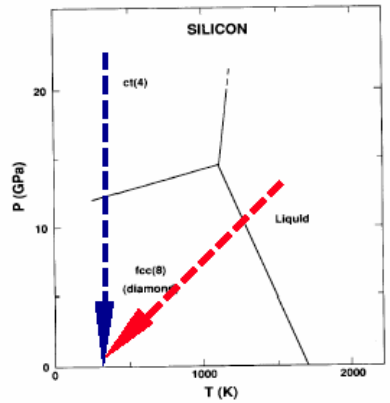
Transition dynamics can be probed across melt and phase boundaries in DAC

Phase diagram of Bi



Rapid resolidification of bcc-Bi across the melt minimum may result in a new metastable phase

Phase diagram of Si



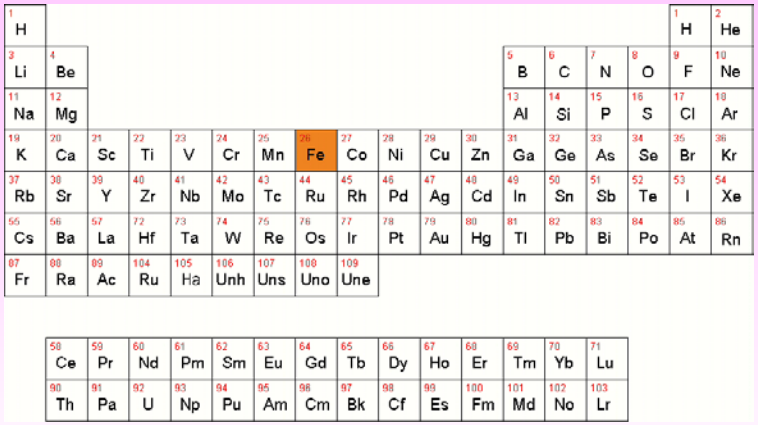
Large difference in bonding of Si may result in the metastability of metallic liquid and solid phases

Modulating DAC is in development at the LLNL

A fast time-resolved x-ray diffraction is a critical enabling technology for the NIF, gas-guns, JASPERS, Z-machine

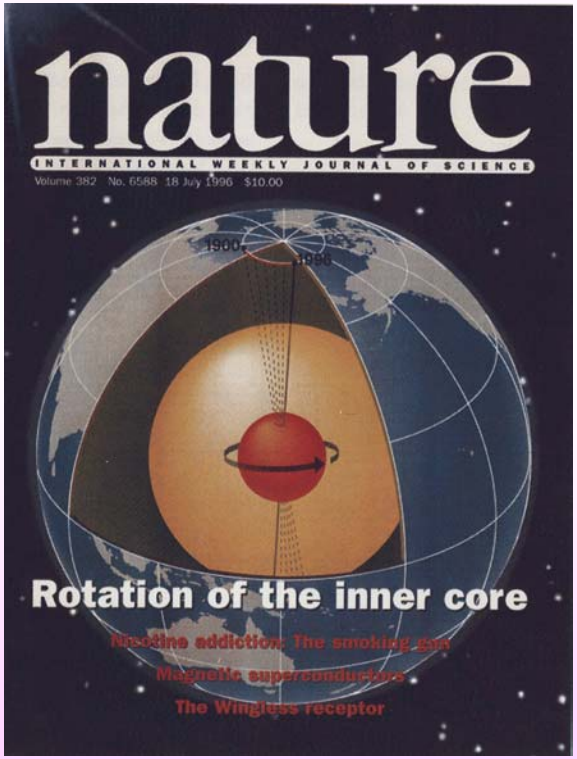
Courtesy of Choong-shik Yoo, LLNL

High-Pressure Behavior of Fe
NEW FINDINGS, PREDICTIONS, SURPRISES



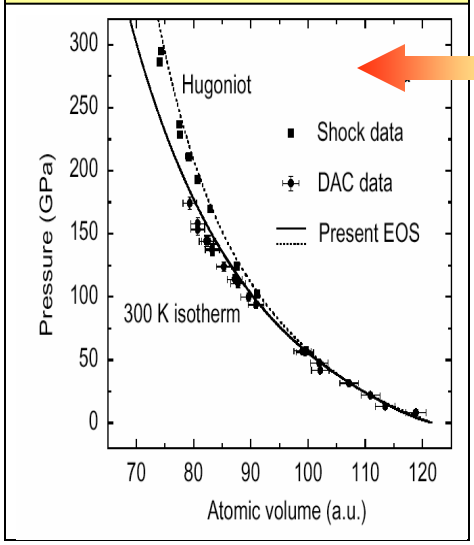
iron

- **High *P-T* polymorphism**
  [Ma *et al.*, to be published]
- **Strength/rheology/elasticity**
  [Singh *et al.* (1998); Merkel et al. to be published]
- **Structural changes in liquid**
  [Sanloup *et al.* (2000)]
- **Magnetic properties: superconductivity**
  [Shimizu *et al.* (2001); Steinle-Neumann et al. (2002); Mazin and Singh (2002)]
- **Pressure-induced reactions**
  FeO, FeH, Fe(Xe)?, Fe(K) ?
  [s -> d transition in K]
  [Parker et al. (1996); Caldwell et al. (1997)]

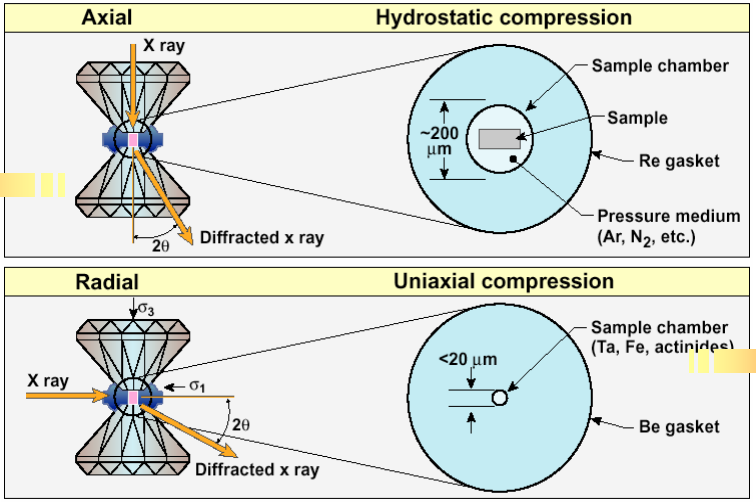


A sub-μm high energy x-ray beam at the APS enables us to determine elastic properties of stockpile materials with high accuracy

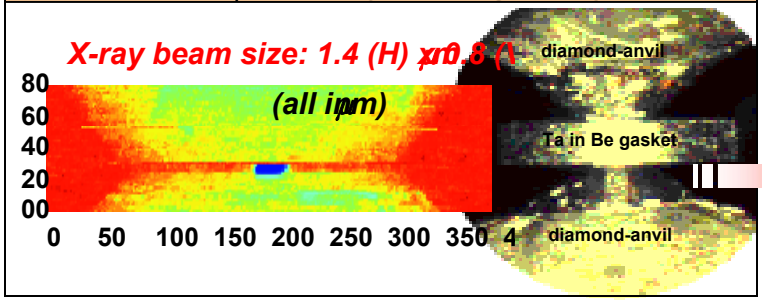
EOS of Ta



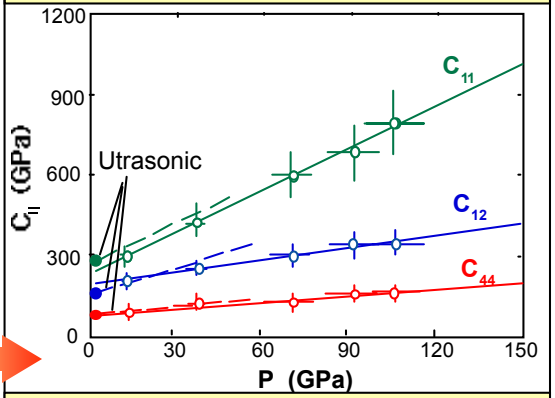
Stress & Angle-resolved X-ray diffraction



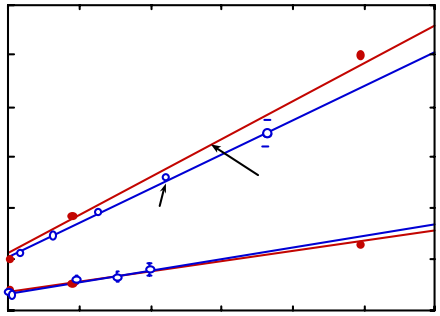
Sub-μm x-ray tomography



Elastic constants (C_{ij}) of Ta



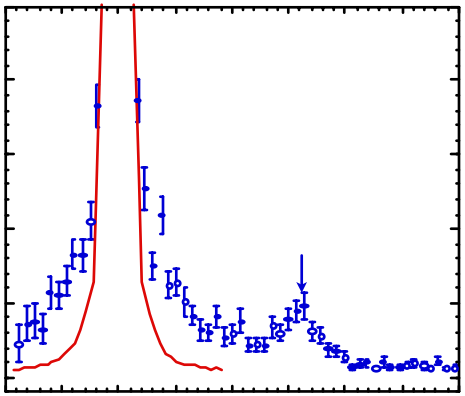
Bulk (B) and shear (G) moduli



Courtesy of Choong-shik Yoo, LLNL

High resolution x-ray at the APS enables us to investigate phonons and electronic structures of f- and d-band transition metals

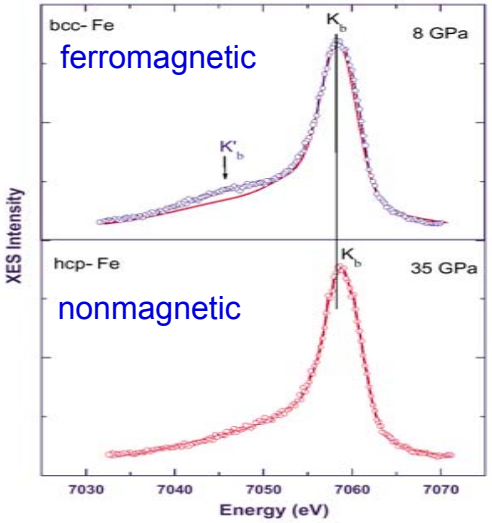
High resolution
Inelastic x-ray scattering



- Phonon dispersion curve
- Sound velocity
- Thermodynamic properties

From the APS

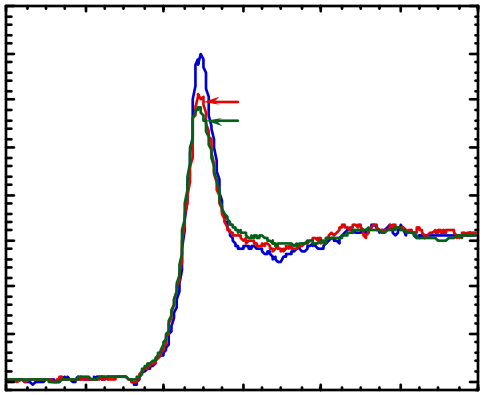
Fine structure of K-edge
X-ray emission



- Valence density of state
- Electronic structure
- Magnetism

From the APS

Near and extended edge
X-ray absorption



- Conduction density of state
- Local structure
- Volume collapse

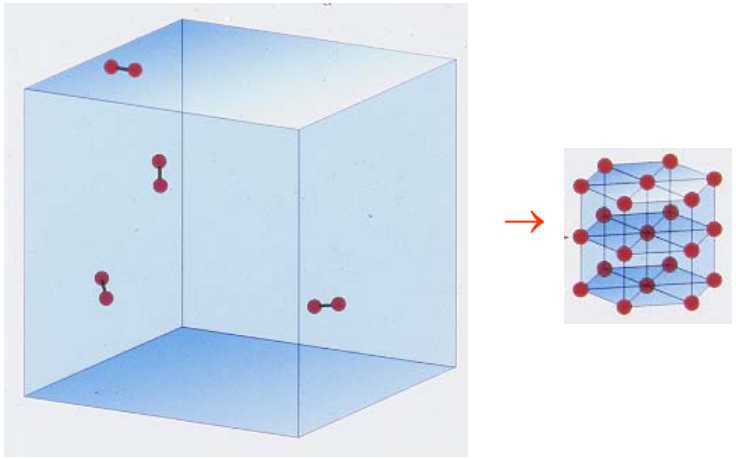
From the NSLS

Volume collapse transitions occurring in many f-band metals, Pr and Pu alike, are electronic in nature, critical to understand the Stockpile performance

Courtesy of Choong-shik Yoo, LLNL

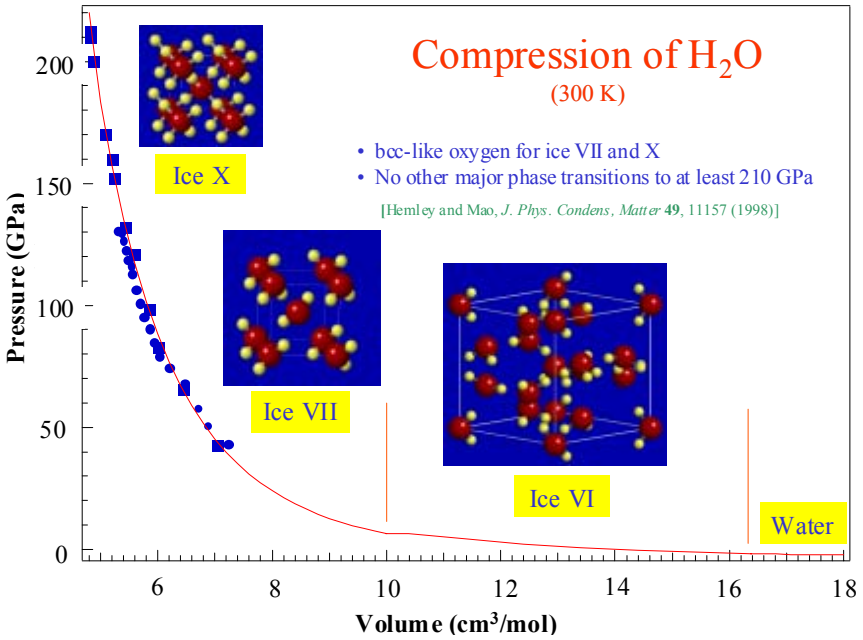
FUNDAMENTAL TRANSFORMATIONS

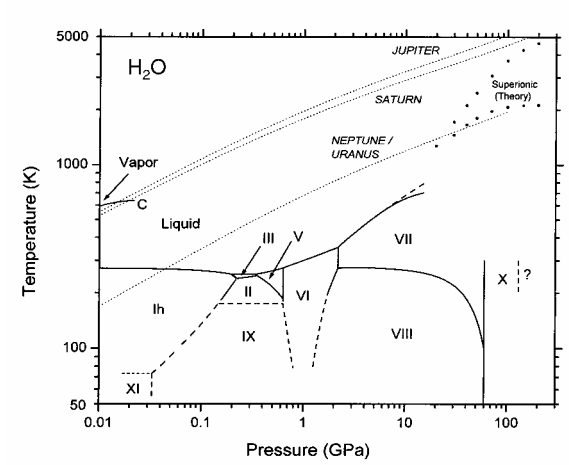
HYDROGEN



- Dissociation/metallization in solid?
- High-temperature superconductor?
- Liquid ground state?
- Transitions in dense fluid?

Structure/bonding/dynamics of hydrogen from neutron diffraction



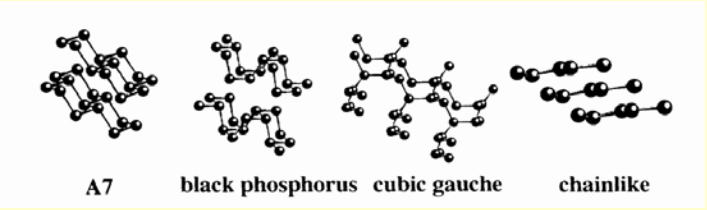


- High-pressure structures (H positions)?
- Metastable transitions (amorphs, liquid)?

New Phases of Nitrogen

EXPLORING THE PHASE DIAGRAM

- **Polymeric phases?**



[McMahan and LeSar (1985), Martin & Needs (1986); Mailhiot et al. (1992)]

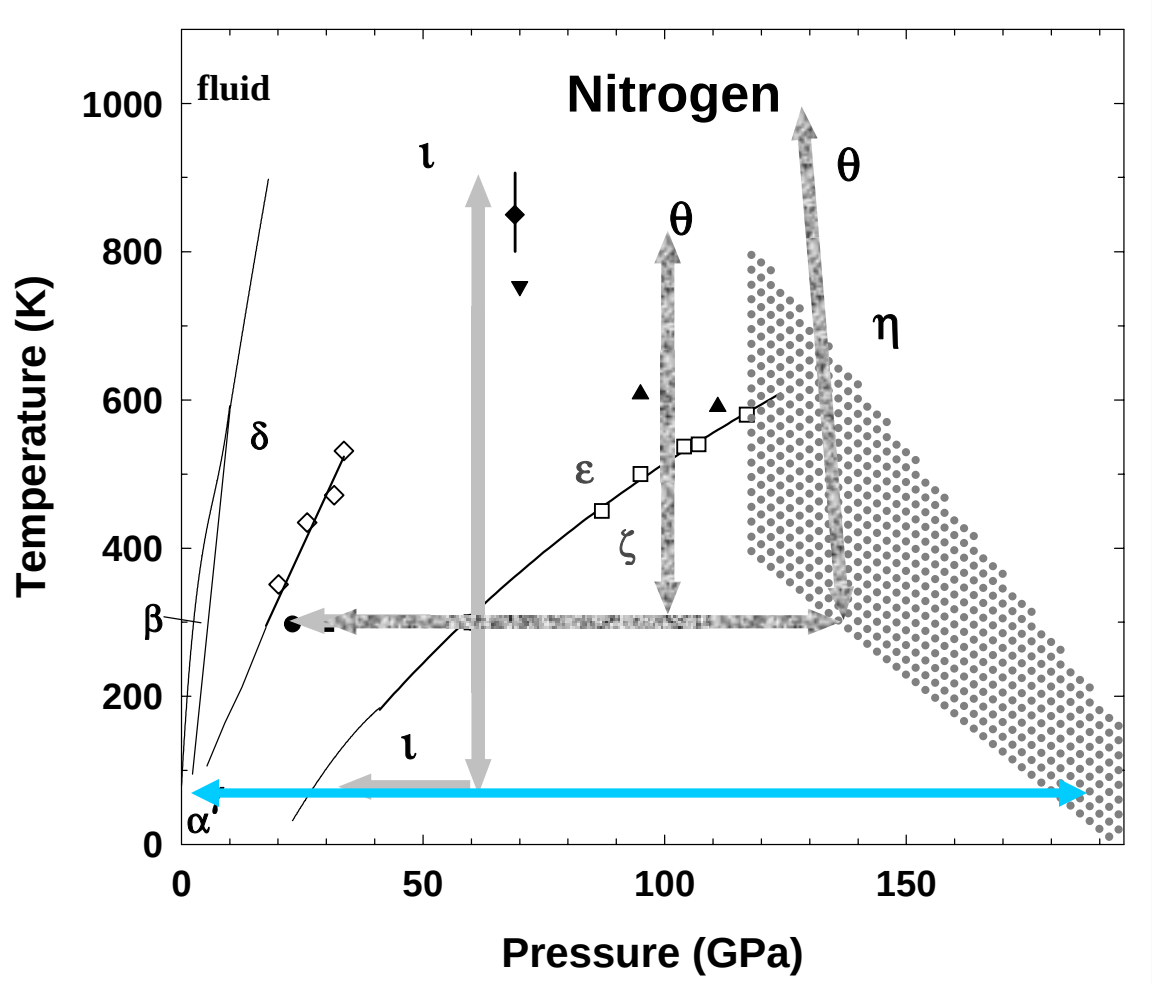
- **New molecular phases?**

Polynitrogen: N_4, N_{10}, $N_5^+N_5^-$?
(~1.9 g/cm^3, 12 GPa for δ-N_2)
[Fau et al., JPC **106**, 4639 (2002)]

- **Quenchable/recoverable?**

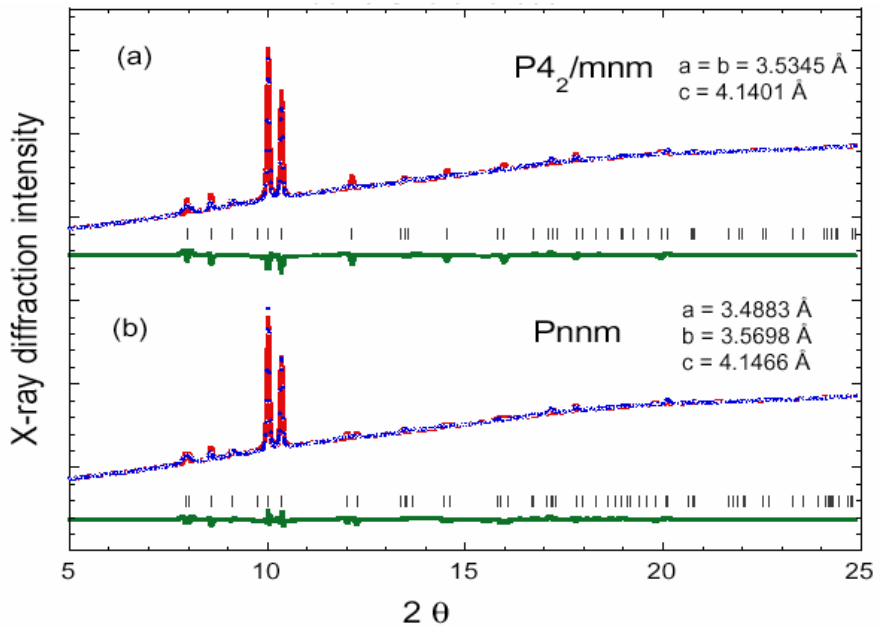
[Eremets *et al., Nature* **411**, 170 (2001)]

[Gregoryanz *et al.*, *Phys. Rev. Lett* , (2001)]



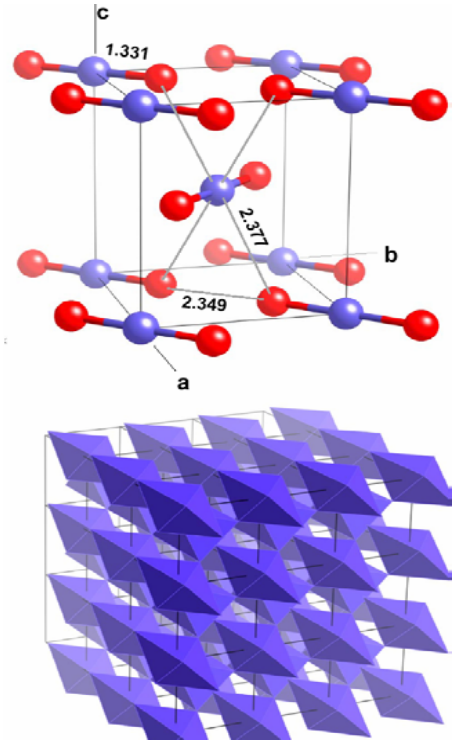
Highly intense high energy x-ray at the APS enables us to characterize crystal structures of low-Z HE and low-symmetry Pu

Angle-resolved x-ray diffraction of CO_2 at high P, T: a major detonation product



A small distortion, < 1 %, of the lattice can be accurately determined *in-situ* at high P,T

Crystal structure of CO_2 that resembles the SiO_2 -stishovite



Courtesy of Choong-shik Yoo, LLNL

Academic participation in technical review process of classified research

- Peer-reviewed publications in classified journals:
  - DP-Labs. Classified journals
  - Q-cleared experts from universities may participate in peer-reviews process
- External reviews:
  - DOE/NNSA Campaigns reviews
  - UC committee for national security
  - JASON review
- Internal reviews at all levels of laboratory:
  - Laboratory/Departmental/Division levels
  - Q-cleared external review committee

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  - Clearly define boundaries
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Clearly define boundaries

Success Story

--benefits researchers, students, and scientific programs of both sides

- Classified research: e.g., *Pu-EOS above ambient pressure, U above 100 GPa*
  - Rules and accountability
  - No university collaboration, but strong synergy

- Unclassified research:e.g., *H_2-EOS at any pressure*
  - No rules are required
  - Mostly scientifically driven

Problems

--when definitions are vague, collaboration withers

- Unclassified, sensitive research: *HE research, simulants, critical technologies, etc.*
  - Boundaries are ill defined
  - University collaborations are vulnerable and threatened by personal liability

Obstacles of classified research activities impact on collaborations

- Limited access to cutting-edge national facilities
  - Classification issues: Raw data vs. classified data
  - Publication issues
  - Materials issues: Safety of radioactive materials
- Hasting political remedies often limiting classified research practices
  - Security shut-downs
  - Polygraphs
- Excessive rules causing difficulties in recruitment and retention of the first-rate scientists and counter productive to
  - Computers
  - **FN and FN from sensitive countries**
  - Limited opportunities for career change of classified researcher
  - Stagnation of research activities

Expanding Successful Models of Academic/DP Interactions

- Direct collaborations with universities *via*
  - ASCI (theory)
  - SSAAP (experimental)

- Collaborations at large-scale national facilities
  - Synchrotron: HP-CAT/APS, CDAC, ALS, NSLS, SSRL, etc.
  - Neutron: LANSCE/LANL, SNS/ONL
  - Laser: NIF/LLNL, Omega/UR

- Exchange and training of future laboratory workforce

- Consultation by Q-cleared academic experts on critical subject areas